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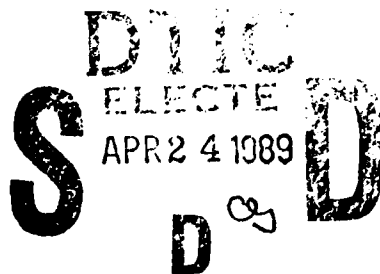
Density-Gradient Theory of Electron Transport in Semiconductors

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DENSITY-GRADIENT THEORY OF ELECTRON TRANSPORT IN SEMICONDUCTORS

1. Introduction.

For a detailed understanding of the physics and engineering of semiconductor devices a macroscopic or continuum description involving the diffusion-drift current equations is often used¹. This description, while having a wide range of applicability, has become increasingly limited in its usefulness as the temporal and spatial scales of state-of-the-art devices have continued to be reduced. The inadequacy of the diffusion-drift description in the new regimes is commonly (although usually implicitly) ascribed to a failure of continuum approximations² and, consequently, microscopic approaches, e.g., Boltzmann or Liouville equations, are widely pursued^{3,4}. In fact, however, continuum approximations often continue to be met in these regimes and it is rather the specific physical (constitutive) assumptions made by the standard diffusion-drift description which are violated. In Ref. 5 and in this report a continuum description which rectifies one of the primary failures of the standard diffusion-drift theory — its inability to account for quantum effects — is developed. The key to this description is a generalization of the equation of state of the electron gas allowing the internal energy of the gas to depend not only on the gas density but also on the density gradient.

Because we are interested in applying a continuum description on smaller spatial scales than are normally addressed by the usual diffusion-drift description, the question of continuum assumptions is an important one. Moreover, a simple example suggests that in fact such assumptions are frequently not met. In an inversion layer in silicon (a situation in which quantum confinement effects are manifested) a typical electron density is $1 \times 10^{18} \text{ cm}^{-3}$ and one would expect a continuum theory would be applicable only over space dimensions large compared to $10 \text{ nm} [(1 \times 10^{18} \text{ cm}^{-3})^{-1/3}]$. Since the inversion layer itself is on the order of 10 nm thick, it follows that a continuum theory cannot be used to

describe the density profile across the inversion layer. Similar arguments suggest that other important device situations involving quantum effects, e.g., tunneling devices or quantum wells, have this same difficulty with continuum assumptions as well. In all such cases, of course, the implication is that microscopic theory must be used instead.

It thus appears that a continuum description of electron transport in semiconductors which contains quantum effects is an impossibility because the spatial scales over which interesting quantum phenomena act seem to be non-macroscopic. Fortunately, it turns out that there are many situations where it is possible to weaken the continuum assumptions and thereby to mitigate this judgement. One way of doing this involves "planar-averaging" and is possible because often in applications, e.g., the inversion layer, we require high resolution in the theory in one dimension only. By restricting the class of volumes over which continuum averages are taken to be flat, "pancake-like" regions rather than regions of arbitrary shape, we can effectively decrease the average "spacing" between electrons in the direction normal to the large faces of the "pancake." In this way, we enhance our ability to describe rapid variations in this normal direction at the expense of a decrease in the in-plane resolution. A second way of weakening continuum assumptions is to trade off temporal resolution for increased spatial resolution (in all directions), thus describing phenomena in time-average only.⁶

Given that a continuum description of the electron density (in a planar-averaged or time-averaged sense or as in Ref. 6) is possible on the small spatial scales of interest, how is such a theory developed? As alluded to above, both direct macroscopic developments and microscopic derivations are possible. The former approach is that of classical field theory⁷ and the specific methods for developing higher-order theories such as the density-gradient description of this report are due to Toupin⁸ and to Green and Rivlin.⁹ In brief, this approach involves postulating a simple model, determining the constraints

imposed by general balance laws and thermodynamic principles and then, within these constraints, selecting the particular material behavior by a choice of constitutive equations (in our work, simple linear response functions). For the latter, alternative approach of a microscopic derivation the starting point is classical or quantum statistical mechanics and the macroscopic equations are obtained using averaging and truncation procedures. This approach has been used previously to derive density-gradient type theories in both a classical framework using the Chapman-Enskog expansion¹⁰ and for the quantum case using the Wigner function.¹¹ To some extent the macroscopic and microscopic approaches are complementary in that the former has advantages of simplicity and generality while the latter can provide additional physical insight and give explicit formulae for material coefficients appearing in the continuum equations (in terms of "fundamental" constants). As noted earlier, in this report we employ the macroscopic approach.

As in Ref. 5, two methods of implementing the macroscopic approach are pursued. The first is a variational development which follows the work of Toupin⁸ and whose prime advantage is its simple, known starting point. Its main disadvantage is that it applies only to non-dissipative situations and thus only to semiconductors in (static) equilibrium. The second method of obtaining the macroscopic equations is a balance law approach due to Green and Rivlin⁹ and it is capable of handling dissipative situations. Additional details concerning these two approaches and a thorough discussion of their relative merits has been given by Tiersten and Bleustein.¹²

Finally, in this report we extend the balance law derivation given in Ref. 5 to incorporate the effects of macroscopic inertia. This extension is needed because electron gas inertia, usually negligible in semiconductor transport problems, is frequently significant in situations where quantum effects are important. Because it turns out that no chemical potential formulation of the theory (as given in Ref. 5) is possible, at least in principle,

when inertia is non-negligible, in this report, we give the complete theory (including boundary conditions) in the more fundamental and widely applicable form involving the electron gas pressure. However, because of the usefulness of a chemical potential formulation, we also present the equations in this form with the effects of inertia approximated so as to be valid under most circumstances.

The density-gradient theory of electron transport in a semiconductor as developed herein can be expected (and, to some extent, has been shown¹³⁻¹⁵) to be of considerable use in modeling semiconductor devices in which quantum effects are important. The primary reason for this is that the continuum description is much simpler than the existing alternatives which are fully microscopic.^{2,4} By including quantum effects to lowest order only, the macroscopic description is simple enough that other important parts of real device modeling problems such as scattering, electrostatics and boundary effects can be analyzed without great increases in computational expense.

2. Variational Development of Density-Gradient Theory in the Static Case

When no dissipation is present, as in a semiconductor in (static) equilibrium, one can obtain the governing equations of macroscopic systems from a variational principle (Lagrangian). For the situation of interest in this report, the variational approach has several advantages. Most importantly, the known functional form of the internal energy density of the electron gas, i.e., with a density-gradient dependence, is a direct input to the analysis. The starting point in the alternative balance law approach (Sec. 3) is much less clear and, in fact, can best be determined from the variational principle. An additional advantage of the variational approach is that, because we discuss a fluid, one of the boundary conditions is much more evident.

For the variational principle, we assume the existence of an electron gas with charge density ρ^e and an internal energy per unit charge of ϵ^e . Following Toupin we then postulate the variational principle

$$(2.1) \quad \delta \int_V \rho^e \epsilon^e dV = \int_V F_j^1 \delta y_j dV + \int_S F_j^2 \delta y_j dS + \int_S F_j^3 D(\delta y_j) dS + \oint_C F_j^4 \delta y_j ds$$

where S denotes an arbitrary surface enclosing a fixed volume V and C consists of edges in the surface S , i.e., lines of intersection of smooth portions of S . In (2.1) and throughout this report we employ Cartesian coordinates in indicial notation with repeated indices being summed (Einstein summation convention). The y_j are the present (or Eulerian) coordinates of the electron gas, δ indicates variation holding the reference (or Lagrangian) coordinates $^7 X_K$ of the gas fixed and D signifies the normal derivative. The quantities F_j^1 , F_j^2 , F_j^3 and F_j^4 are generalized forces representing all "external" interactions. The precise physical origin of these forces is immaterial for the variational principle which focuses entirely on the reaction of the gas. In our case, these external interactions are electrostatic forces and forces exerted by interfaces.

The central assumption of density-gradient theory is that the internal energy of the conduction electron gas in a semiconductor is dependent on both the density and the density-gradient, viz.,

$$(2.2) \quad \epsilon^e = \epsilon^e(\rho^e, \rho_{,i}^e)$$

where $\rho_{,i}^e \equiv \frac{\partial \rho^e}{\partial y_i}$. Given this, we can use (2.1) to determine the equations which govern the system. This is accomplished by inserting (2.2) into (2.1) and, by a series of

manipulations, putting the left-hand side of (2.1) into the form of a sum of integrals like those appearing on the right-hand side of (2.1). The assertion that the variations δy_j and $D(\delta y_j)$ are independent and arbitrary then leads directly to the governing equations.

As a first step in this process, by changing variables from present to reference coordinates and then back, we transform the left-hand side of (2.1) according to

$$(2.3a) \quad \delta \int_V \rho^e \epsilon^e dV = \delta \int_{V_0} \rho_0^e \epsilon^e dV_0 = \int_{V_0} \rho_0^e \delta \epsilon^e dV_0 = \int_V \rho^e \delta \epsilon^e dV ,$$

where ρ_0^e and V_0 are the density and volume, respectively, in reference coordinates.

Inserting (2.2) into (2.3a) we then have

$$(2.3b) \quad \delta \int_V \rho^e \epsilon^e dV = \int_V \rho^e \left[\frac{\partial \epsilon^e}{\partial \rho^e} \delta \rho^e + \frac{\partial \epsilon^e}{\partial \rho_{,i}^e} \delta(\rho_{,i}^e) \right] dV .$$

It is readily shown that

$$(2.3c) \quad \delta \rho^e = -\rho^e (\delta y_i)_{,i} ,$$

and, using the relation, $\delta X_{L,i} = -X_{L,j} (\delta y_j)_{,i}$, that

$$(2.3d) \quad \delta(\rho_{,i}^e) = -\rho_{,i}^e (\delta y_j)_{,j} - \rho^e (\delta y_j)_{,ji} - \rho_{,j}^e (\delta y_j)_{,i} ,$$

and therefore (2.3b) may be re-expressed as

$$(2.4) \quad \delta \int \rho^e \epsilon^e dV = - \int_V \left[(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho} - \frac{\eta_i^e}{\rho^e} \rho_{,i}^e \right] (\delta y_j)_{,j} dV + \int_V \frac{\eta_i^e}{\rho^e} \rho_{,j}^e (\delta y_j)_{,i} dV \\ + \int_V \eta_i^e \delta_{kj} (\delta y_j)_{,ki} dV.$$

where $\eta_i^e \equiv -(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho_{,i}}$ is identified in Sec. 3 as the "double-pressure" in the electron gas.

Now, as pointed out by Green and Rivlin⁹, the last integral in (2.4) could include an arbitrary tensor $M_{[ki]j}$ which is antisymmetric in its first two indices (as indicated by the brackets) since $M_{[ki]j} (\delta y_j)_{,ki} = 0$. Such a term would have no consequences in the variational principle — it does no work — and hence would not enter either the differential equations or the boundary conditions which describe the system (although as shown in Ref. 9 it can be important in formulating the latter). However, this term would enter into the expression for the stress tensor (see Sec. 3). And because in the present work the density-gradient effects arise microscopically from quantum mechanics, we will make a particular selection of the $M_{[ki]j}$ which leads to the stress tensor being in agreement with that obtainable from quantum mechanics.¹¹ It is to be emphasized that this selection has no macroscopic consequences and is made entirely on the basis of a microscopic argument. The particular choice we make for the $M_{[ki]j}$ is reflected in the integrand of the last integral of (2.4). The expression $\eta_i^e \delta_{kj}$ may be written as $\eta_{(ki)j}^e + \eta_{[ki]j}^e$ where $\eta_{(ki)j}^e \equiv \frac{1}{2}[\eta_i^e \delta_{kj} + \eta_k^e \delta_{ij}]$ is symmetric on the first two indices while $\eta_{[ki]j}^e \equiv \frac{1}{2}[\eta_i^e \delta_{kj} - \eta_k^e \delta_{ij}]$ is antisymmetric. The latter quantity, irrelevant from a macroscopic standpoint as explained above, is the particular antisymmetric tensor, i.e., with no additional $M_{[ki]j}$, which we select so as to obtain agreement with quantum mechanical results.

Next, using integration by parts and the divergence theorem, the integrals on the right side of (2.4) can be transformed as follows,

$$(2.5a) \quad \int_V \left[(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho^e} - \frac{\eta_i^e}{\rho^e} \rho_{,i}^e \right] (\delta y_j)_{,j} dV = \int_S n_j \left[(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho^e} - \frac{\eta_i^e}{\rho^e} \rho_{,i}^e \right] \delta y_j dS \\ - \int_V \left[(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho^e} - \frac{\eta_i^e}{\rho^e} \rho_{,i}^e \right]_{,j} \delta y_j dV ,$$

$$(2.5b) \quad \int_V \frac{\eta_i^e}{\rho^e} \rho_{,j}^e (\delta y_j)_{,i} dV = \int_S n_i \frac{\eta_i^e}{\rho^e} \rho_{,j}^e dS - \int_V \left[n_i \frac{\eta_i^e}{\rho^e} \rho_{,j}^e \right]_{,i} \delta y_j dV ,$$

$$(2.6) \quad \int_V \eta_i^e \delta_{kj} (\delta y_j)_{,ki} dV = \int_S n_j \eta_i^e (\delta y_j)_{,i} dS - \int_V \eta_{i,j}^e (\delta y_j)_{,i} dV ,$$

where n_i is the outward normal vector to the surface S . Equation (2.6) can be further transformed by a second integration by parts to obtain

$$(2.7) \quad \int_V \eta_i^e \delta_{kj} (\delta y_j)_{,ki} dV = \int_V \eta_{i,j}^e \delta y_j dV - \int_S D_i [n_j \eta_i^e] \delta y_j dS - \int_S n_i \eta_{i,j}^e \delta y_j dS \\ + \int_S n_j \eta_i^e D(\delta y_j) dS + \int_S D_i [n_j \eta_i^e \delta y_j] dS ,$$

where D_i is the surface gradient operator defined by $D_i \equiv \frac{\partial}{\partial y_i} - n_i D$. We remark that this result depends on the order in which the two integrations of (2.6) and (2.7) have been performed. However, it is readily shown that reversing the order of integration is equivalent to including an additional term of the form $M_{[ki]j}$ in (2.4) and thus is macroscopically irrelevant. Because (2.7) is the expression which leads to consistency with quantum mechanics, had the reverse order of integration been used we would simply have selected the tensor $M_{[ki]j}$ differently (not $\eta_{[ki]j}^e$ as above) so as to again obtain (2.7). Finally, using the surface divergence theorem we can rewrite $\int_S D_i [n_j \eta_i^e \delta y_j] dS$ as

$\oint_C \mathbf{m}_i \cdot \mathbf{n}_j \eta_i^e \delta \mathbf{y}_j ds$, where \mathbf{m}_i is the unit vector binormal to the edges C . This combined with (2.7) and (2.5) allow (2.4) to be fully transformed into a sum of integrals like those on the right-hand side of (2.1). With some further algebra and the assumption that the variations $\delta \mathbf{y}_j$ and $D(\delta \mathbf{y}_j)$ are arbitrary and independent (which implies that each integrand must vanish), we obtain the following equations:

$$(2.8a) \quad F_j^1 = \left[(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho^e} + \rho^e \left(-\frac{\eta_i^e}{\rho^e} \right)_{,i} \right]_{,j} - \left[\frac{\rho^e_{,j} \eta_i^e}{\rho^e} \right]_{,i}$$

$$(2.8b) \quad F_j^2 = -\mathbf{n}_j \left[(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho^e} - \frac{\eta_i^e \rho^e_{,i}}{\rho^e} \right] - \mathbf{n}_i \rho^e \left(-\frac{\eta_i^e}{\rho^e} \right)_{,j} - D_i(\mathbf{n}_j \eta_i^e)$$

$$(2.8c) \quad F_j^3 = \mathbf{n}_i \mathbf{n}_j \eta_i^e$$

$$(2.8d) \quad F_j^4 = [\mathbf{m}_i \mathbf{n}_j \eta_i^e] = \frac{1}{2} [\mathbf{m}_i \mathbf{n}_j \eta_i^e + \mathbf{m}_j \mathbf{n}_i \eta_i^e]$$

where the convention $[A] \equiv A^+ - A^-$ is used to signify the discontinuity in A across the edge C whose binormal vector \mathbf{m}_i points from the minus side of the edge to the plus side. The second equality in (2.8d) follows from the facts that $\mathbf{m}_i \mathbf{n}_j \eta_i^e - \mathbf{m}_j \mathbf{n}_i \eta_i^e = \frac{1}{2} \mathbf{m}_i \mathbf{n}_k \epsilon_{mki} \epsilon_{mjr} \eta_r^e$ (ϵ_{mki} is the usual permutation symbol), that $\mathbf{m}_i = \epsilon_{ijk} s_j \mathbf{n}_k$ (s_j is the unit vector tangent to the edge C) and that η_i^e does not depend on the normal vector \mathbf{n}_i . Lastly, in addition to (2.8b–d) we have another boundary condition which arises because both $\delta \mathbf{y}_j$ and $D(\delta \mathbf{y}_j)$ are continuous across interfaces. That both of these quantities are continuous implies that $(\delta \mathbf{y}_j)_{,j}$ and, from (2.3c), that $\delta \rho^e / \rho^e$ are also continuous. In order for the latter to be true, we must thus impose the additional boundary condition

(2.9)

$$[\rho^e] = 0$$

on all semiconductor boundary-value problems solved within density-gradient theory.

Equations (2.8) are the governing equations of the gas with (2.8a) being the differential equation of equilibrium (force balance) and (2.8b-d) representing boundary and edge conditions. However, for these equations to be practically useful it is necessary that the physical meaning of the F_j^k be identified (e.g., F_j^1 turns out to be the electrostatic force), a task not readily accomplished in the variational approach.^{9,12} These identifications are much more apparent in the balance law approach discussed in Sec. 3.

One final point concerning the variational results relates to the derivation of Sec. 3 using the balance law approach of Green and Rivlin. As noted previously the latter approach, while having a number of advantages, has the drawback that its starting point is not readily known. The known relation $\epsilon^e = \epsilon^e(\rho^e, \rho_{,i}^e)$, which was an input to the variational principle [(2.2)], is a consequence in the balance law approach if the starting point is chosen properly. An added benefit of the variational approach is that it may be used to determine this starting point. In particular, the balance law approach requires an expression for the rate at which gradient effects ("double-tractions") do work on the electron gas. For consistency with the variational principle, this expression must take the form

$$(2.10) \quad \int_S n_j \eta_i^e v_{j,i}^e dS$$

where v_j^e is the velocity of the electron gas.

3. Balance Law Derivation of Density-Gradient Theory

In obtaining macroscopic equations using the balance law approach of Green and Rivlin⁹, the underlying model of the system must be made more explicit than was necessary for the variational principle. For this report, we model the semiconductor as two interacting continua, one being an electron gas which flows with velocity v_i^e inside the other, a rigid solid (lattice). (For simplicity we omit the hole continuum which had been included in Ref. 5). The charge density in the former is denoted ρ^e while in the latter it is ρ^i and we allow no interchange of charge between the two continua through ionization or recombination processes. Because the electron gas and the lattice are charged, they can interact with one another through the electrostatic field E_i . In addition, we permit the gas and solid to interact through a (resistive) drag force E_i^e which impedes the flow of the electron gas through the solid. Finally, the most important interactions for this work (as seen in Sec. 2) concern how the electron gas interacts with itself. First, as in standard diffusion-drift theory,¹⁶ we permit neighboring elements of gas to interact across their surface of separation through a gas pressure p^e (or equivalently a stress tensor $-p^e \delta_{ij}$). Secondly, we allow a more general interaction through a second-rank tensor called the "double-traction" Δ_{ij}^e (also called a double-force^{5,12} or a dipolar traction⁹) in order that the internal energy of the gas be density-gradient dependent. Actually, a gas which interacts through a double-traction is energetically sensitive to the individual components of the strain-gradient and, for our case, this is overly general. In particular, we would like the dependence to be on the components of the strain-gradient, only in the specific combination that is the density-gradient. To specialize the theory in this way, among other things, it is necessary that an additional stress contribution be specified which is not expressible as a pressure; therefore, in association with the double-traction Δ_{ij}^e , we permit an additional surface traction t_i^e in the analysis also. We remark that the distinction

between double-tractions and traction (or pressure or stress) is that tractions do work when the gas moves over a distance whereas double-tractions do work when the gas itself is strained.

The equations of electrostatics and the conservation laws of charge and linear momentum as applied to the foregoing semiconductor model are readily formulated. In integral form they are

$$(3.1a) \quad \int_S n_i D_i dS = \int_V (\rho^e + \rho^i) dV ,$$

$$(3.1b) \quad \oint_C E_i ds_i = 0 ,$$

$$(3.1c) \quad \frac{\partial}{\partial t} \int_V \rho^e dV + \int_S n_i v_i^e \rho^e dS = 0 ,$$

$$(3.1d) \quad - \frac{\partial}{\partial t} \int_V \rho^e \alpha^e v_i^e dV = \int_S (-n_i p^e + t_i^e - \alpha^e \rho^e n_j v_j^e v_i^e) dS + \int_V \rho^e (E_i + E_i^e) dV = 0 .$$

where D_i is electric displacement, α^e is the charge to mass ratio of an electron, C is a closed contour and S is the surface of a fixed volume V . Because α^e is constant,¹⁷ the mass balance equation for the electron gas contains no additional information beyond the charge balance equation (3.1c) and can therefore be omitted. In addition to (3.1) and most importantly for purposes of this report, we have thermodynamic equations, the first being an expression for the conservation of energy in the system. For this equation, as noted at the end of Sec. 2, it is necessary that we have an expression not only for the rates at which the pressure p^e and the associated surface traction t_j^e in the gas do work but also for the rate of working of the double-traction Δ_{ij}^e . The most general form for the latter is $\Delta_{ij}^e v_{j,i}^e$.

However, as noted above, this general form leads to the internal energy of the gas depending on the individual components of the strain-gradient tensor rather than simply on the density-gradient and so needs to be restricted. As discussed in Sec. 2, how this is accomplished is not very clear in the Green-Rivlin approach but variationally we were able to argue that the correct form should be (2.10). Using a standard argument of Cauchy⁷ which permits t_i^e to be written as $n_i \tau_{ij}^e$ where τ_{ij}^e is the associated stress tensor in the gas, we can re-express Δ_{ij}^e as $n_k \eta_{kij}^e$ where η_{kij}^e is the "double-stress" (or dipolar stress⁹) tensor. In terms of this tensor, the rate-of-working expression (2.10) is obtained if η_{kij}^e is specialized to

$$(3.2) \quad \eta_{kij}^e = \delta_{kj} \eta_i^e.$$

As noted in Sec. 2, we term η_i^e the "double-pressure". As in Sec. 2, an additional tensor antisymmetric on its first two indices ($M_{[ki]j}$) could, in general^{9,12} be added to the above however we exclude this in order that the stress tensor computed here agree with the corresponding quantum mechanical expression.¹¹

Employing (2.10) for the rate at which double-pressure does work on the electron gas we may now write the energy conservation equation as

$$(3.3) \quad \frac{\partial}{\partial t} \int_V (\epsilon - \frac{1}{2} \alpha^e \rho^e v_i^e v_i^e + \rho^e \epsilon^e) dV = \int_S (-p^e n_i v_i^e + n_i \tau_{ij}^e v_j^e + n_j \eta_i^e v_{j,i}^e + \frac{1}{2} \alpha^e \rho^e n_j v_j^e v_i^e v_i^e - n_i v_i^e \rho^e \epsilon^e) dS + \int_V (\rho^e E_i v_i^e + E_i \frac{dP}{dt}) dV.$$

As usual, away from interfaces the field variables are continuous and, by standard arguments,⁷ differential forms of (3.1) and (3.3) may be deduced. These are

$$(3.4a) \quad D_{i,i} = \rho^e + \rho^i ,$$

$$(3.4b) \quad E_i \equiv -\varphi_{,i} ,$$

$$(3.4c) \quad \frac{d^e \rho^e}{dt} + \rho^e v_{i,i}^e = 0 ,$$

$$(3.4d) \quad -\alpha^e \rho^e \frac{d^e v_i^e}{dt} = -p_{,i}^e + \tau_{ji,j}^e + \rho^e (E_i + E_i^e) ,$$

$$(3.4e) \quad \frac{d\epsilon}{dt} + \rho^e \frac{d^e \epsilon^e}{dt} - \left[\frac{p^e}{\rho^e} + \frac{\eta_i^e \rho_{,i}^e}{(\rho^e)^2} \right] \frac{d^e \rho^e}{dt} + \frac{\eta_i^e}{\rho^e} \frac{d^e}{dt} (\rho_{,i}^e) - v_{j,i}^e \left[\tau_{ij}^e + \rho^e \left(\frac{\eta_i^e}{\rho^e} \right)_{,j} \right] - E_i \frac{dP}{dt} = -\rho^e E_i v_i^e .$$

In obtaining (3.4e) we have employed (3.4a)–(3.4d), the material derivatives,

$$(3.5a) \quad \frac{d}{dt} \equiv \frac{\partial}{\partial t} \quad \text{and} \quad \frac{d^e}{dt} \equiv \frac{\partial}{\partial t} + v_i^e \frac{\partial}{\partial y_i} ,$$

and the fact that

$$(3.5b) \quad \left[\frac{d^e \rho^e}{dt} \right]_{,i} = \frac{d^e}{dt} (\rho_{,i}^e) + v_{j,i}^e \rho_{,j}^e .$$

Now, in order that ϵ^e depend only on the density–gradient as desired and not on the individual components of the strain–gradient it is necessary that the coefficient of the term involving $v_{j,i}^e$ in (3.4e) vanish. This can be achieved by selecting the associated stress tensor τ_{ij}^e to be

$$(3.5c) \quad \tau_{ij}^e = -\rho^e \left[\frac{\eta_i^e}{\rho^e} \right]_{,j}.$$

We note that if a term $M_{[ki]j}$ had been included in (3.2) then all equations would be as above except (3.5c) which would contain the additional term $-M_{[ki]j,k}$. As noted previously, this additional term has been assumed zero because (3.5c) is in conformity with an expression derivable from quantum mechanics.¹¹

Equation (3.4e) is commonly called the first law of thermodynamics for the macroscopic system under consideration. The form of this equation permits the second law of thermodynamics to be written as¹⁸

$$(3.6) \quad \frac{d\epsilon}{dt} + \rho^e \frac{d\epsilon^e}{dt} - \left[\frac{p^e}{\rho^e} + \frac{\eta_i^e \rho_{,i}^e}{(\rho^e)^2} \right] \frac{d\rho^e}{dt} + \frac{\eta_i^e}{\rho^e} \frac{d}{dt}(\rho_{,i}^e) - E_i \frac{dP_i}{dt} = T \frac{d\eta}{dt},$$

where T is the temperature and η is the entropy per unit volume. Combining (3.4e) and (3.6) we then have, for a uniform temperature state, the rate of entropy production inequality¹⁸

$$(3.7) \quad \frac{d\eta}{dt} = -\frac{1}{T}(\rho^e E_i v_i^e) \geq 0.$$

Equations (3.4), (3.6) and (3.7) are the differential equations which comprise the general, two-constituent, density-gradient description of a semiconductor. Being 10 equations in 22 unknowns this system is, as is usual for such equations, underdetermined and additional equations must be supplied. The 12 auxiliary equations are the so-called constitutive theory which specifies the material properties of the particular system under consideration. Their functional forms may be deduced from the requirements imposed by

the need to satisfy (3.6) and (3.7). The equations deriving from (3.6) are the recoverable or non-dissipative constitutive equations while those from (3.7) are dissipative. Here we focus on the former.

The form of (3.6) shows that ϵ and, most importantly for this report, ϵ^e have the desired functional forms, i.e.,

$$(3.8a) \quad \epsilon = \epsilon(P_i),$$

$$(3.8b) \quad \epsilon^e = \epsilon^e(\rho^e, \rho_{,i}^e)$$

where the temperature (entropy) dependences have been left implicit. To obtain the recoverable constitutive equations we insert (3.8) into (3.6) and carry out the time-derivatives of ϵ and ϵ^e . Then, from the fact that the time derivatives of ρ^e , $\rho_{,i}^e$, P_i and η are independent and can hold arbitrary values, it must be that their respective coefficients vanish. This results in a set of equations, the recoverable constitutive equations, which may be written

$$(3.9a) \quad P_i = P_i(E_j) \quad \text{or} \quad D_i = D_i(E_j),$$

$$(3.9b) \quad \frac{p^e}{\rho^e} = \rho^e \frac{\partial \epsilon^e}{\partial \rho^e} - \frac{\eta_i^e \rho_{,i}^e}{(\rho^e)^2},$$

$$(3.9c) \quad \frac{\eta_i^e}{\rho^e} = -\rho^e \frac{\partial \epsilon^e}{\partial \rho_{,i}^e},$$

where we note that (3.9c) is in accord with the definition for η_i^e used in Sec. 2. As noted

above, the dissipative constitutive theory arises from (3.8) and, as discussed in Ref. 18, would give rise to a functional relationship for E_i^e . This equation together with (3.8) and (3.9) are the 12 constitutive equations which make the differential system fully determinate.

The final component of the theory, necessary for formulating boundary value problems, is a set of consistent boundary conditions. In the balance law approach, these are obtained by taking appropriate limits of the integral forms of the governing equations.⁷ For example, by applying (3.1a) and (3.1c) to an arbitrary pillbox region encompassing a portion of the interface and taking the limit as the volume collapses to the interface in the usual way, we obtain

$$(3.11a) \quad n_i [D_i] = \sigma ,$$

$$(3.11b) \quad \frac{\partial \sigma}{\partial t} + n_i [\rho^e v_i^e] = n_i [\rho^e v_i^e + \frac{\partial D_i}{\partial t}] = 0 .$$

where $\sigma \equiv \lim_{V \rightarrow 0} \int_V \rho^i dV$ is the usual surface charge density at the interface. In a similar way, by taking an arbitrary closed contour which intersects the interface and taking the limit as it collapses to the interface, from (3.1b) we have

$$(3.11c) \quad [\varphi] = 0 .$$

And, applying the same process to (3.1d) as was applied to (3.1a,b) and assuming that ρ^e remains bounded in the limit (in accord with the above definition of σ) we obtain

$$\begin{aligned}
(3.11d) \quad F_j^e &= n_i [-p^e \delta_{ij} + \tau_{ij}^e - \alpha^e \rho^e v_i^e v_j^e] \\
&= n_j \left[-(\rho^e)^2 \frac{\partial \epsilon^e}{\partial \rho^e} + \frac{\eta_i^e \rho^e}{\rho^e} \right] + n_i \left[-\alpha^e \rho^e v_i^e v_j^e - \rho^e \left[\frac{\eta_i^e}{\rho^e} \right]_{,j} \right]
\end{aligned}$$

where (3.5c), (3.9b) and (3.9c) have been used to obtain the second equality and $F_j^e \equiv \lim_{V \rightarrow 0} \int_V \rho^e E_j^e dV$ is the force exerted by the interface on the electron gas. If this force is important, e.g., in the case of an insulating boundary, a surface thermodynamics like that of Ref. 18 would have to be developed and from it a constitutive equation for F_j^e deduced. We note that (3.11d), when written in equilibrium form (with $v_i^e = 0$), differs from the equilibrium condition (2.8b) derived from the variational principle [apart from differences associated with (2.8d) being a traction condition while (3.11d) is a continuity or interface condition] in that (2.8d) contains the added term $D_i(n_j \eta_i^e)$. Below this difference is resolved, however, first we obtain several conditions arising from the introduction of density-gradient dependence and, consequently, double-traction Δ_{ij}^e into the theory.

The first double-traction condition results from an assumption that the normal component of the double-traction, $n_i \Delta_{ij}^e$, is continuous across interfaces. Rewriting this in terms of double-pressure η_i^e we have the boundary condition

$$(3.12) \quad 0 = [n_i \Delta_{ij}^e] = [n_i n_j \eta_i^e] .$$

This is of the same form as the corresponding variational condition (2.8c) and implies that the normal component of η_i^e is continuous. Because the starting point of the balance law approach, (3.2), did not contain an additional arbitrary tensor $M_{[ki]j}$ [in order to obtain (3.5c)], it cannot also be true in general that the tangential component of η_i^e is continuous. Thus, we assume

$$(3.13a) \quad \bar{r}_i = [\eta_i^e]$$

where \bar{r}_i is a vector tangent to the surface. We note that this condition is not needed for solving boundary value problems (no similar condition arose in the variational approach) and \bar{r}_i may be computed using (3.13a) following the solution of a particular boundary value problem. The computed vector \bar{r}_i represents the reaction of the interface to a tangential double-pressure exerted on it by the electron gas. We further note that, away from edges C, the surface gradient of (3.13a) may be formed [first multiplying (3.13a) by n_j] to obtain

$$(3.13b) \quad D_i(n_j \bar{r}_i) = [D_i(n_j \eta_i^e)] .$$

The last double-traction condition in the theory is across edges C. We demand that the vector $m_i \Delta_{ij}^e$ be continuous and thus have the edge condition

$$(3.14) \quad 0 = [m_i n_j \eta_i^e] = \frac{1}{2} [m_i n_j \eta_i^e + m_j n_i \eta_i^e]$$

where the second equality is reached using the same argument employed in (2.8d).

Condition (3.14) is identical in form to (2.8d). Finally, density-gradient theory has the additional condition obtained from the variational principle in (2.9) that demands that the electron gas density be continuous across interfaces. There is no explicit justification for this condition in the balance law approach; it is simply a kinematic condition.

In summary, the density-gradient description of a semiconductor consists of the differential equations, (3.4), the constitutive equations, (3.8) and (3.9) plus equations for E_i^e and F_i^e , and the consistent boundary and edge conditions, (2.9), (3.11a-d), (3.12) and

(3.14).

With the foregoing balance law development in hand, following Refs. 9 and 12, we can now return to the variational approach and identify expressions for, and thus the physical origins of, the unknown generalized forces F_j^k in (2.8a-d). In particular, comparing (2.8a-d) with the equilibrium forms of (3.4d), (3.11d) with (3.13b), (3.12) and (3.14) we obtain

$$(3.15a) \quad F_j^1 = \rho^e E_j ,$$

$$(3.15b) \quad F_j^2 = F_j^e - D_i(n_j \bar{r}_i) ,$$

$$(3.15c) \quad F_j^3 = 0 ,$$

$$(3.15d) \quad F_j^4 = 0 .$$

We remark that it is the existence of the tangential interface double-pressure \bar{r}_i and the condition (3.13b) which lead to agreement between (2.8b) and (3.11d).

As a final task for this Section we obtain a more useful form of the density-gradient theory, which had been exhibited also in Ref. 5 and which puts the equations in a form much like that of the standard semiconductor equations (diffusion-drift theory). This form is reached by transforming the equations so that they are expressed in terms of a (generalized) chemical potential rather than the gas pressure, stress and double-pressure as above. Such a transformation simplifies the mathematics considerably and, as with the standard theory, provides a physical underpinning for and extends the use of so-called "energy diagrams" frequently used in the qualitative discussion of semiconductor devices to

situations in which quantum effects are important. To use other terminology, it defines the conditions under which a quasi-Fermi level description may be used or, equivalently, shows when a diffusion-drift type description is appropriate. Unfortunately, the chemical potential transformation in either the standard theory or the density-gradient theory is impossible when inertia is non-negligible (and possibly also in the presence of material inhomogeneity), which is often the case when density-gradient (quantum) effects are important. Thus, strictly speaking, when inertial effects are significant it is necessary to deal with the pressure equations directly. Nonetheless, because of the great usefulness of the chemical potential equations, we develop such equations below. These equations will be exact when inertia is negligible and a reasonable approximation for most cases when it is not.

The chemical potential transformation, of course, affects only the equations expressing momentum balance: (3.1d), (3.4d) and (3.11d). For density-gradient theory, this transformation hinges upon the fact that, assuming material homogeneity, from (3.8b) and (3.5c) it is readily shown that

$$(3.16) \quad -r_{ij,i}^e + p_{,j}^e = \rho^e \left[\frac{\partial(\rho^e \epsilon^e)}{\partial \rho^e} + \left[\frac{\eta_i^e}{\rho^e} \right]_{,i} \right]_{,j}.$$

And, consequently, if we define a generalized chemical potential as

$$(3.17) \quad \varphi^{e*} \equiv \varphi^e + \left[\frac{\eta_i^e}{\rho^e} \right]_{,i},$$

where $\varphi^e \equiv \frac{\partial(\rho^e \epsilon^e)}{\partial \rho^e}$ is the usual chemical potential, then using (3.16), (3.4d) may be re-written as

$$(3.18) \quad -\alpha^e \frac{d v_i^e}{dt} = -(\varphi + \varphi^{e*})_{,i} + E_i^e.$$

This equation is particularly simple when inertia is negligible ($\alpha^e \rightarrow 0$). Now, to obtain consistent boundary conditions we of course need an integral form of (3.18). We postulate the following:

$$(3.19) \quad -\alpha^e \frac{\partial}{\partial t} \int_V v_i^e dV - \frac{\alpha^e}{2} \int_S n_i v_j^e v_j^e dS - \alpha^e \int_V v_j^e (v_{i,j}^e - v_{j,i}^e) dV = - \int_S n_i (\varphi + \varphi^{e*}) dS + \int_V E_i^e dV.$$

The difficulty in obtaining boundary conditions from this expression is evident. The third term on the left-side may be infinite in the limit as the pillbox collapses about the interface. It is only in one-dimension, for which this term is zero, that there are no such difficulties. In two or three dimensions the requirement for this term being zero is that the flow be irrotational, a condition which is not in general true. Because of the great usefulness of the chemical potential formulation we assert, however, that in the majority of cases, either one-dimensional or irrotational flows are approximated and that therefore the contribution of this term to the boundary condition is negligible. Granting this assertion, (3.19) then leads to the chemical potential boundary condition

$$(3.20) \quad [\varphi + \varphi^{e*} - \frac{\alpha^e}{2} v_i^e v_i^e] = f^{e*}$$

where $\int_S n_i f^{e*} dS = \lim_{V \rightarrow 0} \int_V E_i^e dV$ and f^{e*} is the force per charge exerted by the interface on the electron gas. As with F_j^e , a functional form for f^{e*} may be obtained by setting up a surface thermodynamics.¹⁸

4. Partial Specification of the Constitutive Theory

In order to make the theory developed in Secs. 2 and 3 concrete, in this Section we present a set of simple constitutive equations which appear to lead to a useful theory.¹³⁻¹⁵ We here discuss only the bulk constitutive equations. The primary equation, of course, is the equation of state of the electron gas; that is, we need to select a particular expression for (2.2). We construct this expression for ϵ^e from two terms, a purely density dependent term $\epsilon_0^e(\rho^e)$ and a term involving both the density and the density-gradient $\epsilon_1^e(\rho^e, \rho_{,i}^e)$ with the latter term vanishing when the density-gradient is zero. The first term must obviously be of the form used in standard diffusion-drift theory. For low densities, this form is that of ideal gas, i.e., with p^e linearly proportional to ρ^e . Selecting

$$(4.1) \quad \epsilon_0^e(\rho^e) = \frac{E_c}{q} - \frac{kT}{q} [\ln(-\rho^e/qN_c) - 1]$$

and using (3.9b) we have, as desired,

$$(4.2a) \quad p^e = -\frac{kT}{q} \rho^e$$

and

$$(4.2b) \quad \phi^e = \frac{E_c}{q} - \frac{kT}{q} \ln(-\rho^e/qN_c) .$$

For the density-gradient dependent term we again would like the lowest order form. Just like with the density term, this is obtained when the double-pressure η_i^e is linearly proportional to the density-gradient $\rho_{,i}^e$. The appropriate form for ϵ_1^e is

$$(4.3) \quad \epsilon_1^e(\rho^e, \rho_{,i}^e) = -\frac{b}{2} \frac{\rho_{,i}^e \rho_{,i}^e}{(\rho^e)^2}.$$

Inserting (4.3) into (3.9c) then yields the linear relationship

$$(4.4a) \quad \eta_i^e = b \rho_{,i}^e$$

and

$$(4.4b) \quad \varphi^{e*} = \varphi^e + \frac{b}{\rho^e} \rho_{,ii}^e - \frac{b}{2} \frac{\rho_{,i}^e \rho_{,i}^e}{(\rho^e)^2}.$$

The coefficient b in (4.3) and (4.4) is a macroscopic material coefficient which characterizes the strength of the density-gradient effect in the electron gas. In Ref. 11, a microscopic formula for b was obtained (subject to specific microscopic assumptions) of the form $b = h^2/(48\pi^2 m^* q)$ where m^* is the effective mass, h is Planck's constant and q is the charge on an electron. Of course, in a macroscopic framework such a coefficient should be experimentally determined.

In addition to the constitutive specification for ϵ_i^e to fully determine the differential equations we require also equations for the electric displacement D_i [(3.9a)] and for the drag force E_i^e . For both we take the simplest form of a linear proportionality:

$$(4.5) \quad D_i = \epsilon_s E_i$$

and

$$(4.6) \quad E_j^e = \frac{v_j^e}{\mu^e}$$

where, as usual, ϵ_s is the electric permittivity of the semiconductor and μ^e is the electron mobility. With assumptions (4.1), (4.3), (4.5) and (4.6) the differential equations are fully specified. All of these equations are familiar except for that expressing momentum balance which is the same (except in the case of material inhomogeneity) in either the pressure (3.4d) or chemical potential formulation (3.14). Written in a diffusion-drift-like form, the momentum balance equation is

$$(4.7) \quad J_i^e \equiv \rho^e v_i^e = -\mu^e \rho^e E_i - D^e \rho_{,i}^e + 2\mu^e b \rho^e \left[\frac{s_{,ij}}{s} \right]_{,i}$$

where J_i^e is the electron current density, $D^e \equiv kT\mu^e/q$ (k is Boltzmann's constant) is the electron gas diffusion constant and, for compactness, we use the variable s defined by $s \equiv \sqrt{-\rho^e}$. The first two terms on the right side are the usual drift and diffusion expressions of the standard transport theory and the third term represents the correction arising from density-gradient (quantum) effects. Consequently, (4.7) may be referred to as a generalized diffusion-drift current equation and the third term, since it arises from the gradient of the generalized chemical potential (3.13), may be called "quantum diffusion." Equation (4.7) has been demonstrated to be in very good agreement with experiments and with microscopic theory in both static¹³ and steady-state^{13,15} applications.

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